



Figure 2

Training Set									ontput
			Control	PURSUIT	Sethoxim	Ghrohosate	Diuron	Foul	Assignment
na022400 02	2	Control	0.99996	0	0.00001	0.00003	0.00002	0.00001	Control
a022400 05	Ŋ	Control	0.99998	0	0	0.00002	0.00003	0.00001	Confro
a030100_06	53	Control	0.99998	0	0	0.00002	0.00003	0.00001	Control
1030100 09	32	Control	0.99998	0	0	0.00001	0.00004	0.00001	Control
030100 11	34	PURSUIT	c	96666.0	0.00004	0.00003	0.00004	0 0000	PIRSIIT
3030100 14	37	PURSUIT		966660	0.0000	0.00004	0 00004	0 0000	PIIPSIIIT
17 0030100	40	PURSUIT		266660	0.00002	0 00003	0 0000	00000	TILISALIA
9030100 19	42	PURSUIT		0.99995	0.0000	00000	00000	00000	TILISALIA
030800	1 6	Control	00000		00000	0000	1000		
5 00000	5 1	1	0.0000	,	0.0000	0.00002	0000	0.0000	50000
000000	81	Semoxyalm	0.0002	0.0000	0.99996	0.0000	0.00001	0.00004	Sethoxydim
030600_10	24	Sethoxydim	0.00002	0.00002	0.99993	0.00002	0.00001	0.00004	Sethoxydim
030600_13	09	Foul	0	0.00004	0.00002	0	0	0.99991	Foul
030600_15	62	Glyphosate	0.00007	0.00004	0.00001	0.99992	0	0.00003	Glyphosate
030600 16	63	Glyphosate	0.0000	0.00004	0.00003	0 99994	_	0 00003	Glynhosate
030600 20	67	Dinon	0 00004	0.00004	00000	_	0 00003	00000	Dinner
na030600_21	88	Diuron	0.00007	0.00004	0 00002	. 0	0.99994	0.00003	Diuron
lest Set									
022400 01	-	Control	0.99998	0	0	0.00002	0.00003	0.00001	Control
na022400 03	ო	Control	96666.0	0	0.00001	0.0001	0.00002	0.00001	Control
022400 04	4	Control	0.99998	0		0 00000	0 00003	0 00001	Control
022400 08	۵.	Control	0 00007		00000				Control
0000000	1 0		00000		0.000	00000		,	
075400 07	٠.	Control	0.33330			0.00002	0.0003	L0000.0	Control
022400 08	20	Control	0.99997	0	0.00001	0.0000	0.00001	0.00001	Control
022400 09	a	PURSUIT	0	0.02733	0	0.01224	0	900000	Unknown
022400 10	6	PURSUIT	0,00086	0.00118	•	0.34361	0	0.00002	Unknown
na022400 11	F	PURSUIT	0.00085	0.00141	0	0.27197	0	0.00002	Unknown
022400 12	12	PURSUIT	0.00016	0.0025		0.12513	0	0.00003	Unknown
022400 13	13	PURSUIT	0.00013	0.00259		0.12979	0	0.00003	Unknown
022400 14	14	PURSUIT	0.00013	0.00238		0.13242		0.00003	Unknown
022400 15	5	PURSUIT	_	0.10029		0.00586	0 0000	0000	Improve
na022400 16	16	PURSUIT	0.00005	0.00469		0.06222		0.00004	linknown
022400 17	17	TIISHID	0 00114	0.00127		20808		00000	Imknown
na022400 18	8	PIRSIIT	0 0004	0.00139		0 27002		20000	Impromen
022400 19	5	THESTIL	0 00048	0.00185		0.18992		00000	linknoum
022400 20	2 2	TILESTIT	0.00244	0000		0.35054		20000	Introduct
2400 34	i	FILIPOLITY				0000	•	20000	Olivino I
0022400		FILEGUIA	0.000	0.0006	•	0.34762		0.00002	uwouxuo.
0052400 52	3 :	TORSO!	0.00040	0.00146	•	0.454/9	>	0.00002	OUKDOWN
022400 23	2	PURSUIT	0.00086	0.00123	•	0.3072	0	0.00002	Unknown
030100 01	24	Control	0.99996	0	0	0.00002	0.00005	0.00001	Control
030100_02	52	Control	0.99997	0	0	0.00001	0.00238	0.00001	Control
1030100 03	28	Control	0.99997	0	0	0.00001	900000	0.00001	Control
030100 04	27	Control	96666.0	c	0 0000	c	0 00001		Control
20 000000	i é							,	5

					1				
Training Set			Control	PURSUIT	Sethoxim	Glyphosate	Diuron	Foul	Assignment
na030100 07	30	Control	0.99998	0	0	0.00002	0.00002	0.00001	Control
na030100 08	31	Control	0.99996	0	0.00002	0	0.00001	0.00001	Control
na030100 10	33	PURSUIT	0	0.99996	0.00001	0.00003	0.00005	0.00002	PURSUIT
na030100 12	32	PURSUIT	0	0.99996	0.00001	0.00003	0.00004	0.00002	PURSUIT
na030100 13	36	PURSUIT	0	0.99996	0.00002	0.00004	0.00004	0.00002	PURSUIT
na030100 15	38	PURSUIT	0	0.99994	0.00003	0.00003	0.00005	0.00002	PURSUIT
na030100_16	39	PURSUIT	0	0.99995	0.00002	0.00003	0.00004	0.00002	PURSUIT
na030100 18	41	PURSUIT	0	0.99995	0.00002	0.00004	0.00004	0.00002	PURSUIT
na030100 20	43	PURSUIT	0	0.9999	0.00005	0.00003	0.00008	0.00003	PURSUIT
na030100_21	44	PURSUIT	0	0.99995	0.00004	0.00004	0.00003	0.00002	PURSUIT
na030100 22	42	PURSUIT	0	0.99995	0.00002	0.00003	0.00004	0.00002	PURSUIT
na030600_12	29	Sethoxydim	0.00005	0.0003	0.99701	0	0.00003	0.00003	Sethoxydim
na030600 14	61	Glyphosate	0.00006	0.00004	0.00002	0.99994	0	0.00003	Glyphosate
na030600 17	64	Glyphosate	0.00005	0.00005	0.00003	0.99993	0	0.00003	Glyphosate
na030600 18	65	Fou	0	0.00007	0.00003	0	0.00001	0.99993	Foul
na030600_19	99	Diuron	0.00034	0.00003	0.00002	0	0.99992	0.00003	Diuron
na030600_22	69	Diuron	0	0.00005	0.00003	0	0.99989	0.00004	Diuron
na030600 23	20	Diuron	0.00065	0.00014	0.00043	0	0.92715	0.00011	Diuron
na030600_24	7	Diuron	0.00002	0.00005	0.00003	0	0.99993	0.00003	Diuron
Training Set									
na022400 02	7	Control	0.99996	0	0.00001	0.00003	0.00002	0.00001	Control
na022400_05	ιO	Control	0.99998	0	0	0.00002	0.00003	0.00001	Control
na030100_06	59	Control	0.99998	0	0	0.00002	0.00003	0.00001	Control
na030100 09	32	Control	0.99998	0	0	0.00001	0.00004	0.00001	Control
na030100_11	8	PURSUIT	0	0.99996	0.00001	0.00003	0.00004	0.00002	PURSUIT
na030100 14	37	PURSUIT	0	0.99996	0.00001	0.00004	0.00004	0.00002	PURSUIT
na030100_17	9	PURSUIT	0	0.99995	0.00002	0.00003	0.00004	0.00002	PURSUIT
na030100_19	45	PURSUIT	0	0.99995	0.00001	0.00004	0.00004	0.00002	PURSUIT
na030600_04	51	Control	0.99993	0	0.00002	0.00002	0.00001	0.00001	Control
na030600_08	S.	Sethoxydim	0.00002	0.00001	0.99996	0.00005	0.00001	0.00004	Sethoxydim
na030600_10	22	Sethoxydim	0.00002	0.00002	0.99993	0.00002	0.00001	0.00004	Sethoxydim
na030600 13	90	Foul	0	0.00004	0.00002	0	0	0.99991	Foul
na030600_15	62	Glyphosate	0.00007	0.00004	0.00001	0.99992	0	0.00003	Glyphosate
na030600_16	83	Glyphosate	0.00006	0.00004	0.00003	0.99994	0	0.00003	Glyphosate
na030600_20	67	Dinron	0.00004	0.00004	0.00002	0	0.99993	0.00003	Diuron
na030600 21	68	Diuron	0.00007	0.00004	0.00002	0	0.99994	0.00003	Diuron

Applicant: Aranibre et al
Serial No: Filed Concurrently Herewith
Tike: Metabohne Profiling Methods Using Chromatographic and SpeData in Pattern Recognition Analysis
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Figure 3b

Applicant: Aranibar et al
Sørial No: Pided Concurrently Herewain
Tulte: Metabolome Profiling Methods Using Chromatographic and Spoctroscopic
Data in Pattern Recognition Analysts
Docket No. 16313-0089
Sheet 5 of 10

SNNS result fil	.e	V1.4-3D				
Training file		na022400				
Test file na040	400					
No. of patterns	:	24				
No. of input un	its:	1080				
No. of output u	mits:	6				
Startpattern:		1				
Endpattern:		24				
Teaching output	included					
Treatment:	1.1 Contro	1				
Target:	1	0	0	0	0	0
Output:	0.99954	0.00045	0.00001	0.00001	0.00001	0.00001
Treatment:	2.1 Contro	1				
Target:	1	0	0	0	0	0
Output:	0.99936	0.00065	0.00001	0.00001	0.00001	0.00001
Treatment:	3.1 Contro		1.10001		1.10001	3.30001
Target:	1	0	0	0	0	0
Output:	0.99951	0.00047	0.00001	0.00001	0.00001	0.00001
Treatment:	4.1 Contro		0.00001	0.00001	0.00001	0.00001
Target:	1	0	0	0	0	0
Output:	0.99963	0.00037	0.00001	0.00001	0.00001	0.00001
Treatment:	5.1 Chlors		0.00001	0.00001	0.00001	0.00001
Target:	0	0	0	0	0	0
Output:	0.00159	0.99843	0	0.00001	0	o l
Treatment:	6.1 Chlors			0.00001		
Target:	0.1 (11015	0	0	0	0	0
Output:	0.00806	0.99165	0	0	0	0
Treatment:	7.1 Chlors					
Target:	0	0	0	0	0	
	-	-				0
Output: Treatment:	0.00334 8.1 Chlors	0.99669	_0	0	0	0
	8.1 Chiors		_	_	_	
Target:		0	0	0	0	0
Output:	0.00014	0.99985	_0	0.00001	0	0
Treatment:	9.1 Chlors		_	_	_	
Target:	0	0	0	0	0	0
Output:	0.00667	0.99376	0	0	0	0
Treatment:	10.1 Imaza		_	_	_	
Target:	0	0	0	0	0	0
Output:	0.00044	0.99955	0	0	0	0
Treatment:	11.1 Imaza					- 1
Target:	0	0	0	0	0	0
Output:	0.00013	0.99987	0	0	0	0
Treatment:	12.1 Imaza					1
Target:	0	0	0	0	0	0
Output:	0.00208	0.99798	0	0.00001	0.00001	0

Figure 4a

SNNS result fil	e	V1.4-3D				- 1
Training file		na022400				
Test file na040						- 1
No. of patterns		24				1
No. of input un	its:	1080				
No. of output u	nits:	6				
Startpattern:		1				- 1
Endpattern:		24				i
Teaching output	included					
Treatment:	13.1 Imaza	methabenz				
Target:	0	0	0	0	0	0
Output:	0.00223	0.99755	0	0	0	0
Treatment:	14.1 Imaza	methabenz				
Target:	0	0	0	0	0	0
Output:	0.06789	0.93484	0	0	0	0
Treatment:	15.1 Sulfu	meturon				
Target:	0	0	0	0	0	0
Output:	0.00046	0.99955	ő	ō	ō	ō
Treatment:	16.1 Sulfu	meturon				
Target:	0	0	0	0	0	0 1
Output:	0.00102	0.999	ō	0.00001	ō	o l
Treatment:	17.1 Sulfu	meturon				
Target:	0	0	0	0	0	0
Output:	0.00194	0.99813	0	0.00001	0	ò
Treatment:	18.1 Sulfu			0.000		
Target:	0	0	0	0	0	0
Output:	0.00013	0.99987	0	0	ō	o I
Treatment:	19.1 Sulfu					
Target:	0	0	0	0	0	0
Output:	0.00014	0.99985	ō	0	o o	ō
Treatment:	20.1 Imaza					
Target:	0	0	0	0	0	0
Output:	0.0018	0.998	a a	0	0	ŏ
Treatment:	21.1 Imaza					
Target:	0	0	0	0	0	0
Output:	0.00031	0.99968	o o	0.00001	o o	ŏ
Treatment:	22.1 Imaza					
Target:	0	0	0	0	0	0
Output:	0.00175	0.99791	o o	Ö	ŏ	ŏ
Treatment:	23.1 Imaza					
Target:	0	DAT	0	0	0	0
Output:	0.00018	0.9998	o o	o o	o o	ŏ
Treatment:	24.1 Imaza					
Target:	0	0	0	0	0	0
Output:	0.06579	0.93074	0	0	0	ŏ
oucput.	0.00077	0.230/4	· .	~	<u> </u>	

Figure 4b

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Rows: Teaching Input; Columns: Classification for Nineteen MOAs (23 Classes, Including "Control" = Untreated Plants, 1 "Spare" Class, and "Unknown" Added by SNNS)

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sansiq #	31	17	e	2	0	-	9	9	9	9	9	m	9	9	9	9	3	9	10	9	12	9	0	0
Ппкпомп	7	0	0	0	0	0	3	0	0	2	4	2	1	2	2	5	-	2	-	0	0	3	0	0
Spare	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SisotiM	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0
Glutamine	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	Ξ	0	0	0
ES_IIS4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	9	0	0	0	0
to_IISq	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-	×	0	0	0	0	0
12_II29	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	-	0	0	0	0	0
Acetamide	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0
она	0	0	0	0	0	0	0	0	0	0	0	0	-	0	-	-	0	0	0	0	0	0	0	0
qenerT nixuA	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0
Auxin-like	0	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0
Ducoupler	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0
PDS	1	0	0	0	0	0	0	0	0	0	0	-	0	0	0	0	0	0	0	0	0	0	0	0
Microtubule	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0
ISd	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Carotenoid	0	0	0	0	0	0	0	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
РКОТОХ	0	0	0	0	0	0	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
нььр	ī	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Necrotic*	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Not Used	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
EPSPS	0	0	0	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ACCase	0	0	e	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SAHA	0	11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Control	27	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
CLASS	Control	AHAS	ACCase	EPSPS	Not Used	Necrotic*	HPPD	PROTOX	Carotenoid	PSI	Microtubule	PDS	Uncoupler	Auxin-like	Auxin Transp	онь	Acetamide	PSII_c1	PSII_c2	PSII_c3	Glutamine	Mitosis	Spare	NoClass

Rows: Teaching Input; Columns: Classifications for Nineteen MOAs (23 Classes, Including "Control" = Untreated Plants, 1 "Spare" Class, and "Unknown" Added by SNNS)

MACA MACA MACA MACA MACA MACA MACA MACA
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MOA Control AHAS AHAS ACCACA EPSPS PS II Necrotic' PROTOX Caroteno PROTOX Caroteno Microtub Microtub Microtub Auxin-Iik Auxin-Iik Auxin-Iik Auxin-Iik Auxin-Iik PSII, Carotub PSII, Caro

Rows: Teaching Input, Columns: Classification as Percentage of Total Plants Tested for Nineteen MOAs (23 Classes, Including "Control" = Untreated Plants, 1 "Spare" Class, and "Unknown" Added by SNNS)

Unknown	9	Г		Т	Т	Т	20	Т	Т	22	19	19	2	33	8	_	83	23	33	2		Т	20
Spare	1	1	t	1	1	1	1	+	1	t	Ť	Ť	T	Ė	Ė		-	Ė	H	Ť	t	t	Ť
sisotiM	l	T	T	T	1		T	T	T	T	T	T	t	t		_		r	h		\vdash	t	20
Glutamine	Г	T			T	Т	T	T	T	T	T	T							T	T	T	25	T
es_usq		Г		Γ		Γ	Γ	Г			T	Π		Г				Г	Г	T	8	T	Г
to_HS¶																		Γ	12	∞		Γ	
PSII_ci		L													-			Г	8	2			П
Acetamide	L				L		L											67					
рнр													11		17		1						
qenerT nixuA	L			_		L	L	L	L		L	Ĺ			20								
94il-nixuA	_							L						29									
Uncoupler	L		L		L								19										
PDS	3											33											
Microtubule	_	_			_		L	L	L		33									_			
ISA	_	L	L	L	L	L	L			19				_									
Carotenoid	_	_			_	L	L	L	8	L		L	_	L	L			L		_	L	_	
хотояч	_		_	_	_	_	L	2	L	L	_	_	_									L	
GTATA	3	_	_	_		L	92	L			L		_	_		1	_			L		L	
Necrotic*	_	_	_	_	<u> </u>	2	_	L	_		_		_	_		_							
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EPSPS		_	_	8	_	<u> </u>	_	L	L	L	_	L				4	_				_		Ш
ACCase			100	ļ.,	_	<u> </u>	_	L		L						4	_			L,	_		Ц
SAHA	-	100		_	_	H	_	L	_	_	-	_	_	_		1	_	_			_	_	니
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CLASS	Control	AHAS	ACCase	EPSPS	Not Used	Necrotic*	HPPD	PROTOX	Carotenoid	ISI	Microtubule	PDS	Uncoupler	Auxin-like	Auxin	Transp	DHD	Acetamide	PSII c1	PSII_c2	PSII 3	Glutamine	Mitosis

Rows: Teaching Input, Columns: Classification as Percentage of Total Plants Tested for Nineteen MOAs (23 Classes, Including "Control" = Unitested Plants, 1 "Spare" Class, and "Unkrnown" Added by SNNS)